

1-Methyl-6-(2-methylphenyl)-1,6-dihydro-3-pyridinecarbonitrile
27531-42-6 | DTXSID60299776

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 118 °C

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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2,5-Cyclohexadien-1-one, 4-[[4-(dimethylamino)phenyl]imino]-

Measured: 134

Predicted: 127

Image not found

Aprindine

Measured: 121

Predicted: 128

Image not found

Michler's ketone

Measured: 179

Predicted: 156

Image not found

Thenalidine

Measured: 96.0

Predicted: 101

Image not found

Pyrimidine, 4-phenyl-

Measured: 56.0

Predicted: 72.3